NASA TECHNICAL MEMORANDUM NASA TM-76203

MODIFICATION OF THE FLOW PASS METHOD AS APPLIED TO PROBLEMS OF CHEMISTRY OF PLANET ATMOSPHERES

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(NASA-TM-76203) MODIFICATION OF THE FLOW PASS METHOD AS APPLIED TO PROBLEMS OF CHEMISTRY OF PLANET ATMOSPHERES (National Aeronautics and Space Administration) 14 p HC A02/MF A01 CSCL 03B G3/91

N81-18973

Unclas 41551

Translation of "Modifikatsiya metoda potokovoy progonki primenitel'no k zadacham khimii planetnykh atmosfer", Academy of Sciences USSR, Institute of Space Research, Moscow, Report Pr-387, 1978, pp. 1-12

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
WASHINGTON, D.C. 20546 AUGUST 1980

STANDARD TITLE PAGE

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA TM-76203		

4. Title and Subtitle	5. Report Date
MODIFICATION OF THE FLOW PASS METHOD AS APPLIED TO PROBLEMS OF CHEMISTRY OF PLANET ATMOSPHERES	August 1980
	6. Performing Organization Code
7. Author(s)	8. Performing Organization Report No.
V. A. Parshev	10. Work Unit No.
9. Performing Organization Name and Address	11. Contract or Grant No.
Leo Kanner Associates Redwood City, California 94063	NASw-3199
	13. Type of Report and Period Covered
12. Sponsoring Agency Name and Address	Translation
National Aeronautics and Space Administration, Washington, D. C. 20546	14. Sponsoring Agency Code

15. Supplementary Notes

Translation of "Modifikatsiya metoda potokovoy progonki primenitel'no k zadacham khimii planetnykh atmosfer", Academy of Sciences USSR, Institute of Space Research, Moscow, Report Pr-387, 1978, pp. 1-12

16. Abstract

Carried out herein is generalization of the flow pass method for a stationary problem of diffusion of a minor component in a stratified medium, with the presence of the force of gravity and chemical reactions.

It is shown that the modified flow pass method, applied to problems of chemistry of planet atmospheres, possesses considerable effectiveness, both in the case when the coefficient of diffusion changes severely in the examined region, and in the case when diffusion is the prevalent process, as compared with chemical reactions, i.e., in the case when a regular pass proves inapplicable, or applicable in a limited interval of the decisive parameters.

17. Key Words (Selected by Author(s))	18. Distribution Statement
	Unlimited-Unclassified

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22.
Unclassified	Unclassified		

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Carried out herein is generalization of the flow pass method for a stationary problem of diffusion of a minor component in a stratified medium, with the presence of the force of gravity and chemical reactions. /2*

It is shown that the modified flow pass method, applied to problems of chemistry of planet atmospheres, possesses considerable effectiveness, both in the case when the coefficient of diffusion changes severely in the examined region, and in the case when diffusion is the prevalent process, as compared with chemical reactions, i.e., in the case when a regular pass proves inapplicable or applicable in a limited interval of the decisive parameters.

The problem of determining the spatial distribution of minor components in the atmospheres of planets amounts to the solution of a system of equations, each of which has the form /3

$$\frac{d\Phi_i}{dz} = p_i - L_i n_i \qquad (1.1)$$

with one of the following typical boundary conditions at the upper boundary:

$$\text{a1/}\quad \Phi_i\big|_{z=z_M} = Q_M \quad \text{—representation of flow,} \qquad (1.2)$$

$$\text{a2/}\quad n_i\big|_{z=z_M} = n_{iM} \quad \text{—representation of concentration}$$

and at the lower boundary:

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*Numbers in the margin indicate pagination in the foreign text.

$$\text{B1/}\quad \Phi_i\big|_{z=0} = Q_0 \qquad \text{—representation of flow,}$$

$$\text{B2/}\quad n_i\big|_{z=0} = (P_i/L_i)\big|_{z=0} \qquad \text{—representation of photo-chemical equilibrium} \tag{1.3}$$

$$\text{B3/}\quad n_i\big|_{z=0} = n_{i0} \qquad \text{—representation of concentration.}$$

Here, n_i is the concentration, and Φ_i is the flow of the component i.

$$\Phi_i = -K\left\{\frac{dn_i}{dz} + \frac{n_i}{H_{cp}} + \frac{n_i}{T}\frac{dT}{dz}\right\} - D_i\left\{\frac{dn_i}{dz} + \frac{n_i}{H_i} + (1+\alpha_i)\frac{n_i}{T}\frac{dT}{dz}\right\}, \tag{1.4}$$

P_i, L_i are the rate of production and the function of particle destruction, k is the coefficient of diffusion, brought about by motion of the medium, D_i is the coefficient of molecular diffusion, H_i, H_{cp} are the scales of the altitudes of the examined component and the medium, respectively, T is the temperature, α_i is the thermodiffusion factor, Z is the altitude reckoned from a certain level (not necessarily from the surface of the planet, 0< ZM), ZM is the upper boundary, and i is the number of the component. /4

Using the method of component breakdown, the problem of many components can be reduced to the sum of the problems of the given type, which makes it possible to examine the problem (1.1)-(1.4) for a single component. Subsequently, the index i will be omitted.

The following boundary value problem corresponds to the differential boundary value problem (1.1)-(1.4):

$$-a_i n_{i+1} + (b_{i-1} + a_{i-1} + \varepsilon_i) n_i - b_i n_{i-1} = d_i, \qquad (2.1)$$

$$F_i = -(a_i n_{i+1} - b_{i-1} n_i) \qquad (2 \le i \le n2-1), \quad (2.2)$$

$$a1/\ F_{n2} = Q_M \ ; \ a2/\ n_{n2} = n_M, \qquad (2.3)$$

$$b1/\ F_1 = Q_c \ ; \ b2/\ n_1 = d_1/\varepsilon_1 \ ; \ b3/\ n_1 = n_0. \quad (2.4)$$

The equation is approximated according to three points on a uniform network, according to Z, in a conservative manner, i is the number of the point in sampling for Z, ε_i is the difference analog of L, d_i is the difference analog of p, and F_i is the difference analog of the flow ϕ.

By bounding our problem by the description of the method of solution of the difference system, according to all questions associated with the derivation and substantiation of the differential equations, as well as the switch to an approximating system of difference equations, we will refer the reader to the appropriate literature (for example, one can find a detailed bibliography on these questions in study [5]).

In order to solve problems of the type (2), the pass method [1] is usually utilized, which possesses great effectiveness and stability and makes it possible to obtain a solution of the problem in a rather broad range of decisive parameters. However, there exists a large class of problems of the described type, when the /5 use of the standard pass method (SP) is not possible, since it leads to a considerable loss of accuracy, for example, in problems of chemistry of planet atmospheres: (*) when the coefficient of diffusion changes severely, i.e., the coefficients a_{i-1}, b_i in (2)

charge in the examined area by several orders; or (**), when the diffusion is a more effective process, as compared with the chemical reactions between the components, and the flow through the boundary is absent, i.e., $a_{i-1}, b_i \gg \varepsilon_i, d_i$ and $F_1 = F_{nz} = 0$. Under these conditions, the total concentration of the component in the examined area is determined by the balance between the total production and destruction, and its altitude distribution is brought about by diffusion. The use of the standard pass method for solving these problems leads to a considerable loss of accuracy, if the order of the relationship of the minimum value of $b_i, \varepsilon_i, d_i, a_{i-1}$ to the maximum value of a_{i-1}, b_i is greater than the number of significant digits with which the computer operates. The flow pass method (PP) [2,3,4] makes it possible to obtain a solution of the problem in both cases (*) and (**), if the flow is determined as $\phi = k\frac{dn}{dz}$.

Given in the present study is a modification of the flow pass method for a flow of a more general type (1.4), which makes it possible to overcome both of the indicated difficulties.

Description of the Algorithm

Thus, we will examine the difference boundary value problem (2.1)-(2.4). For a common pass, we have

$$n_{i+1} = z_i n_i + m_i, \qquad (3.1)$$

$$z_{i-1} = \frac{b_i}{b_{i+1} + a_{i-1} + \varepsilon_i - a_i z_i}, \qquad (3.2)$$

$$m_{i-1} = \frac{d_i + m_i a_i}{b_{i+1} + a_{i-1} + \varepsilon_i - a_i z_i}. \qquad (3.3)$$ /6

The first equation (2), we will write in the form

$$F_i - F_{i-1} = -\mathcal{E}_i n_i + d_i .$$

Expressing $n_{i+1} = -\frac{F_i}{a_i} + \frac{i+1}{a_i} n_i$ from (2.2) and substituting into (3.1), we obtain

$$-F_i + n_i (b_{i+1} - z_i a_i) = m_i a_i . \quad (5)$$

Introducing new coefficients according to the formulas

$$\gamma_i = m_i a_i \; ; \; \alpha_i = b_{i+1} - z_i a_i , \quad (6)$$

we will write (5) in the form

$$-F_i = -\alpha_i n_i + \gamma_i . \quad (7)$$

From (7) and (4), excluding n_i, we obtain the recurrent relationship for the flow

$$F_i = \frac{\alpha_i}{\alpha_i + \mathcal{E}_i} \cdot F_{i-1} + \frac{d_i \alpha_i - \mathcal{E}_i \gamma_i}{\alpha_i + \mathcal{E}_i} .$$

From (6), we obtain the expressions for Z_i, m_i:

$$z_i = \frac{b_{i+1} - \alpha_i}{a_i} \; ; \; m_i = \gamma_i / a_i .$$

From the first equation in (3), we obtain the recurrent relationship for n_i:

$$n_{i+1} = \frac{b_{i+1} - \alpha_i}{a_i} n_i + \frac{\gamma_i}{a_i} \quad (8)$$

The recurrent relationships for α_i, γ_i are obtained from (6), (3.2), and (3.3):

$$\alpha_i = b_{i+1} \frac{\alpha_{i+1} + \varepsilon_{i+1}}{\alpha_{i+1} + a_i + \varepsilon_{i+1}},$$

$$\gamma_i = a_i \frac{d_{i+1} + \gamma_{i+1}}{\alpha_{i+1} + a_i + \varepsilon_{i+1}}. \qquad (9)$$

With regard for (9), expression (8) takes on the form

$$n_{i+1} = \left(b_{i+1} n_i + d_{i+1} + \gamma_{i+1}\right) / \left(\alpha_{i+1} + \varepsilon_{i+1} + a_i\right).$$

The final formulas for the direct pass have the form

$$\alpha_i = b_{i+1} \cdot \frac{\alpha_{i+1} + \varepsilon_{i+1}}{a_i + \alpha_{i+1} + \varepsilon_{i+1}} \; ; \; \gamma_i = a_i \frac{d_{i+1} + \gamma_{i+1}}{a_i + \alpha_{i+1} + \varepsilon_{i+1}}, \qquad (10.1)$$

$$a1/ \quad \alpha_{nz} = 0 \; ; \; \gamma_{nz} = Q_M, \qquad (10.2)$$

$$a2/ \quad \alpha_{nz} = b_{nz} \; ; \; \gamma_{nz} = a_{nz} \cdot n_M \qquad (10.3)$$ /1

Reverse pass is carried out according to the formulas

$$n_{i+1} = a_i \cdot \frac{b_{i+1}}{\varepsilon_{i+1} + \alpha_{i+1}} n_i + \frac{d_{i+1} + \gamma_{i+1}}{a_i + \varepsilon_{i+1} + \alpha_{i+1}},$$

$$F_{i+1} = \frac{\alpha_{i+1}}{\varepsilon_{i+1} + \alpha_{i+1}} F_i + \frac{d_{i+1}\alpha_{i+1} - \varepsilon_{i+1}\gamma_{i+1}}{\varepsilon_{i+1} + \alpha_{i+1}},$$

$$b1/ \quad F_1 = Q_0 \; ; \; n_1 = (\gamma_1 + Q_0)/\alpha_1, \qquad (11)$$

$$b2/ \quad n_1 = d_1/\varepsilon_1 \; ; \; F_1 = (\alpha_1 \cdot d_1/\varepsilon_1) - \gamma_1,$$

$$b3/ \quad n_1 = n_0 \; ; \; F_1 = \alpha_1 \cdot n_0 - \gamma_1.$$

The obtained formulas, as easily noted, are similar to the formulas of flow pass, given in [1]; therefore, they may be

called the algorithm of the modified flow pass (MPP).

The stability of the recurrent relationships given above is evident.

Discussion of the Method

We will give reasons which show that the calculations according to the given scheme prove more accurate than those which are carried out by the traditional pass method.

Insofar as the coefficients a_i, b_i, ε_i, and d_i are positive, the pass coefficients α_i, $\gamma_i > 0$, and, thus, the sums of the positive magnitudes stand both in the numerator and in the denominator of the expressions (10), and, although the absolute error in the sum is made up of the absolute errors of the terms, the relative error does not increase, insofar as the moduli of the magnitudes in the numerator and denominator increase, while the accumulation of the error (relative) during division and multiplication does not have such catastrophic consequences as during subtraction.

If d_i, $\varepsilon_i \ll a_{i-1}$, b_i and $\alpha_{nz} = 0$; $\gamma_{nz} = 0$, then the method of mathe- /8
matical induction may be used to show that $\alpha_{i-1} \leq \varepsilon_i$ and $\gamma_{i-1} \leq \sum_{k=1}^{i} d_k$, i.e., magnitudes of a single order take part in the determination of α_i, γ_i, although only as sums, and the relative error does not increase.

These reasons show that the modified flow pass is free from the above-indicated difficulties, which occur during the solution of problems of chemical kinetics by normal pass.

For illustration, we will examine two models of the problem. The first is described by the following system of equations

$$\text{(A)} \qquad \begin{aligned} &\frac{d\Phi}{dz} = 0, && \Phi = \mathcal{D}\left(\frac{dn}{dz} + n\right); \\ &n\big|_{z=c} = 1, && \mathcal{D} = \exp(\beta z); \\ &\Phi\big|_{z=z_M} = 0, && 0 \leq z \leq 20; \end{aligned}$$

where $\beta>0$ is the parameter of the problem.

There exists an accurate solution of the problem, which has the form

$$n = \exp(-z).$$

The second problem is formulated using the following system of equations

$$(B)\qquad \frac{d\Phi}{dz} = E(1-n), \quad \Phi = \frac{dn}{dz} + n,$$
$$\Phi\big|_{z=0} = 0; \quad \Phi\big|_{z=zM} = 0, \quad 0 \le z \le 20.$$

where the coefficient of diffusion is assumed as equal to 1, $E \ll 1$, $ZM=20$. The asymptotic solution of this problem, with the condition $ZM \cdot E \ll 1$, has the form

$$n = n_0 \exp(-z), \text{ where } n_0 = ZM.$$

For these problems, in accordance with what has been set forth above, approximating difference equations were written, which were solved both by the method of the standard pass and by the method of the modified flow pass. A computer, operating with 12-digit numbers, was utilized for the solution.

Problem (A) was solved with various values of the parameter β in the coefficient of diffusion in a uniform network with a spacing $\Delta Z=0.1$. It turned out that the method of the standard pass, with $\beta<2$, provides a solution of the problem which differs by less than 2% from the analytical solution, but with $\beta>2$, the solution differs considerably from the analytical solution (fig. 2). /9

The method of the modified flow pass provides a solution which

coincides, with an accuracy of up to 2% for all β (fig. 1).

Problem (B) was solved with various values of E in the very same network. It was found that, with $E<10^{-10}$, the solutions for the standard pass and the modified flow pass coincide, with an accuracy of up to 5%, but with $E>10^{-7}$, these solutions differ from the asymptotic solution (fig. 3), and only with $E<10^{-7}$ do all three solutions coincide—that obtained according to the standard pass up to 10%, and that obtained according to the modified flow pass with an accuracy of up to 4% (fig. 4).

With $E<10^{-10}$, the solution by the method of the standard pass is impossible to find (the system becomes confluent for the computer), while the modified flow pass provides a solution with extremely small E, for example, a solution was obtained with $E=10^{-70}$ (fig. 4).

The results given above show the effectiveness of the method of the modified flow pass during the solution of problems of the described type, for example, those associated with the chemistry of planet atmospheres. It combines within itself both the advantages of the standard pass, namely efficiency and a small volume of required storage, and the advantage of methods which utilize a double length of the computer number—namely, high accuracy of solution.

In conclusion, the author thanks V. A. Krasnopol'skiy for his detailed discussion of the study.

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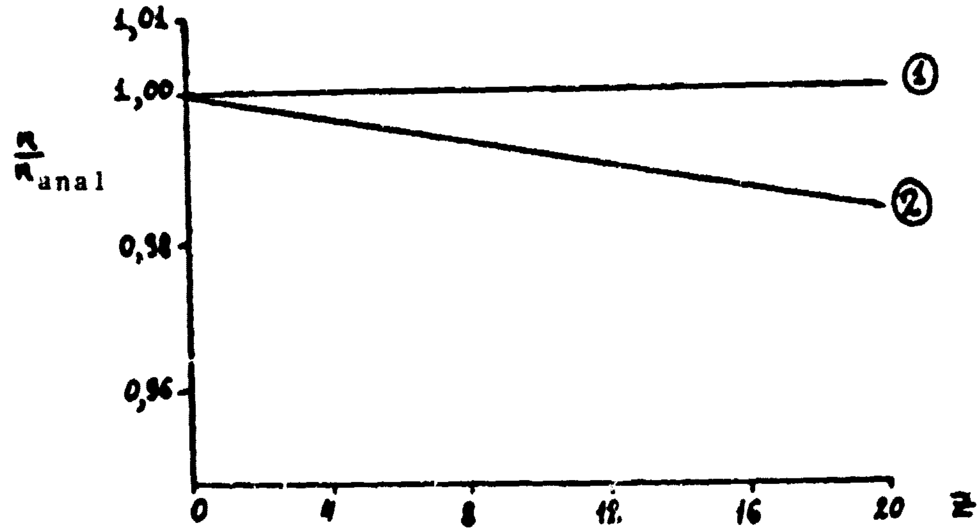

Fig. 1. Dependence of relationship (n/n_{anal}) on the coordinate Z. (1) $n=n_{anal}$; (2) n is the solution of the problem by the method of the modified flow pass and standard pass with $\beta<2$.

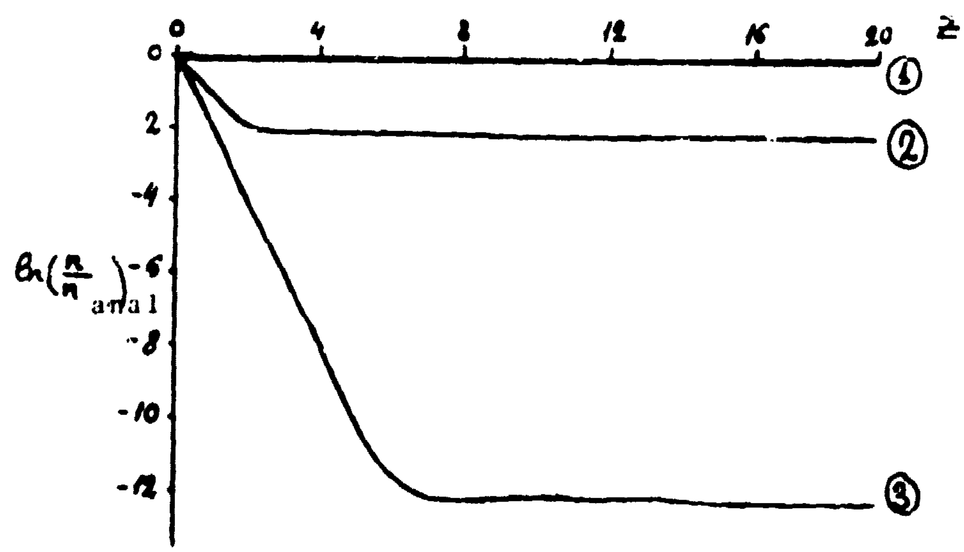

Fig. 2. Dependence of magnitude of $\ln(n/n_{anal})$ on the coordinate Z for problem (A) by the method:
(1) Modified flow pass for all β; (2) Standard pass with $\beta=2.5$; (3) Standard pass with $\beta=3$.

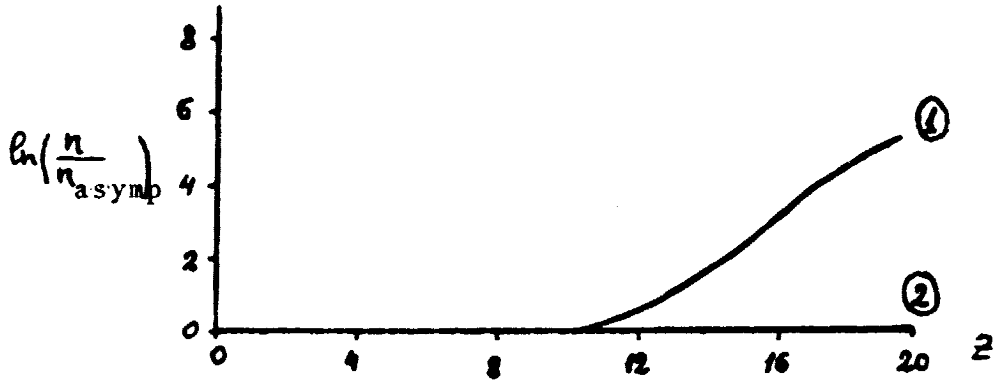

Fig. 3. Dependence of magnitude of $\ln(n/n_{asymp})$ for problem (B) on the coordinate Z:

① $E=10^{-5}$; solutions by modified flow pass and standard pass methods coincide;

② Asymptotic solution and solutions by methods of modified flow pass and standard pass with $E=10^{-10}$ coincide.

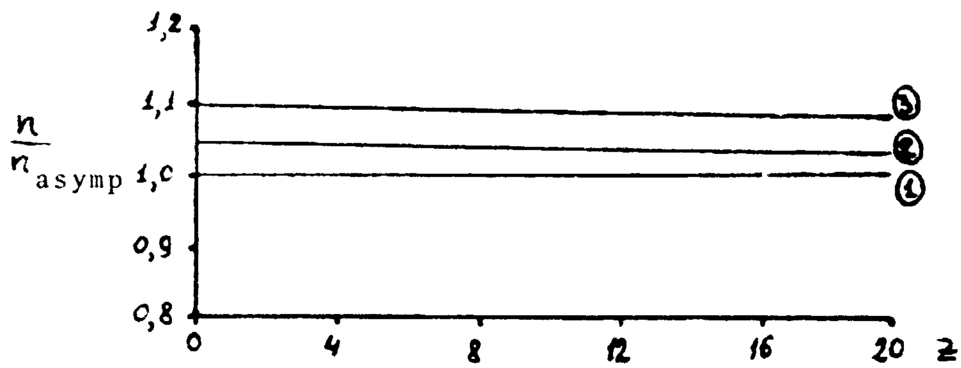

Fig. 4. Dependence of magnitude of (n/n_{asymp}) on coordinates Z for problem (B): ① Asymptotic; ② Modified flow pass with $10^{-8} \geq E \geq 10^{-70}$; ③ Standard pass with $E=10^{-10}$.